Computational Models in the Materials World
- We are nearly there….

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Standard Form 298 (Rev. 8-98)
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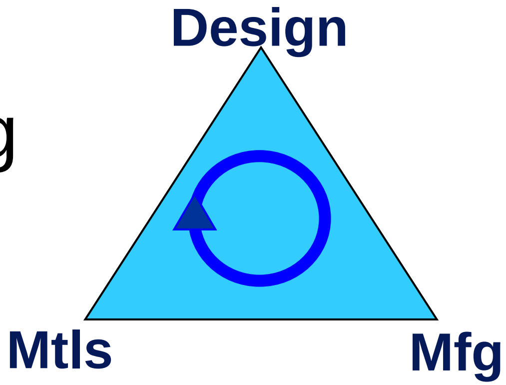
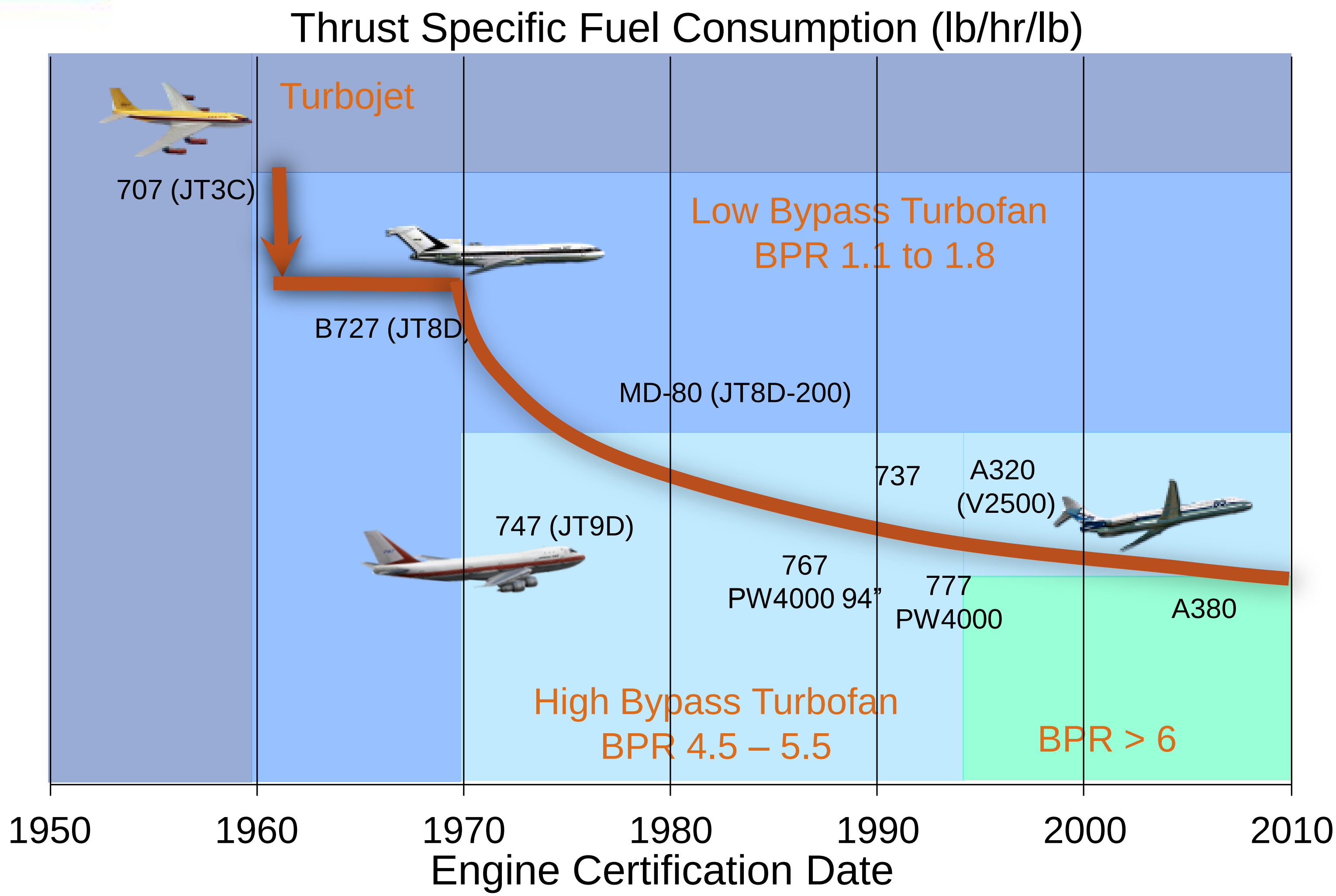
Engineering Materials Today

- Materials are critical for every engineered product
- Traditionally materials were developed by trial and error processes, separate from application requirements
- Materials are currently defined by static specifications based on empirical data
- Challenge and opportunity of Computational Materials Engineering is the linking of Materials, Manufacturing Processes and Component Designs



No Technical Data per the EAR and ITAR

Evolution of System Efficiency



Propulsion History

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Propulsion Innovations Enabled by Materials and Processing Technology

DS blades, Cast &Wrought disks, 1st Gen Thermal Spray TBC coatings

1st Gen SC blades, 1st Gen PM disk, 1st Gen EB-PVD TBC

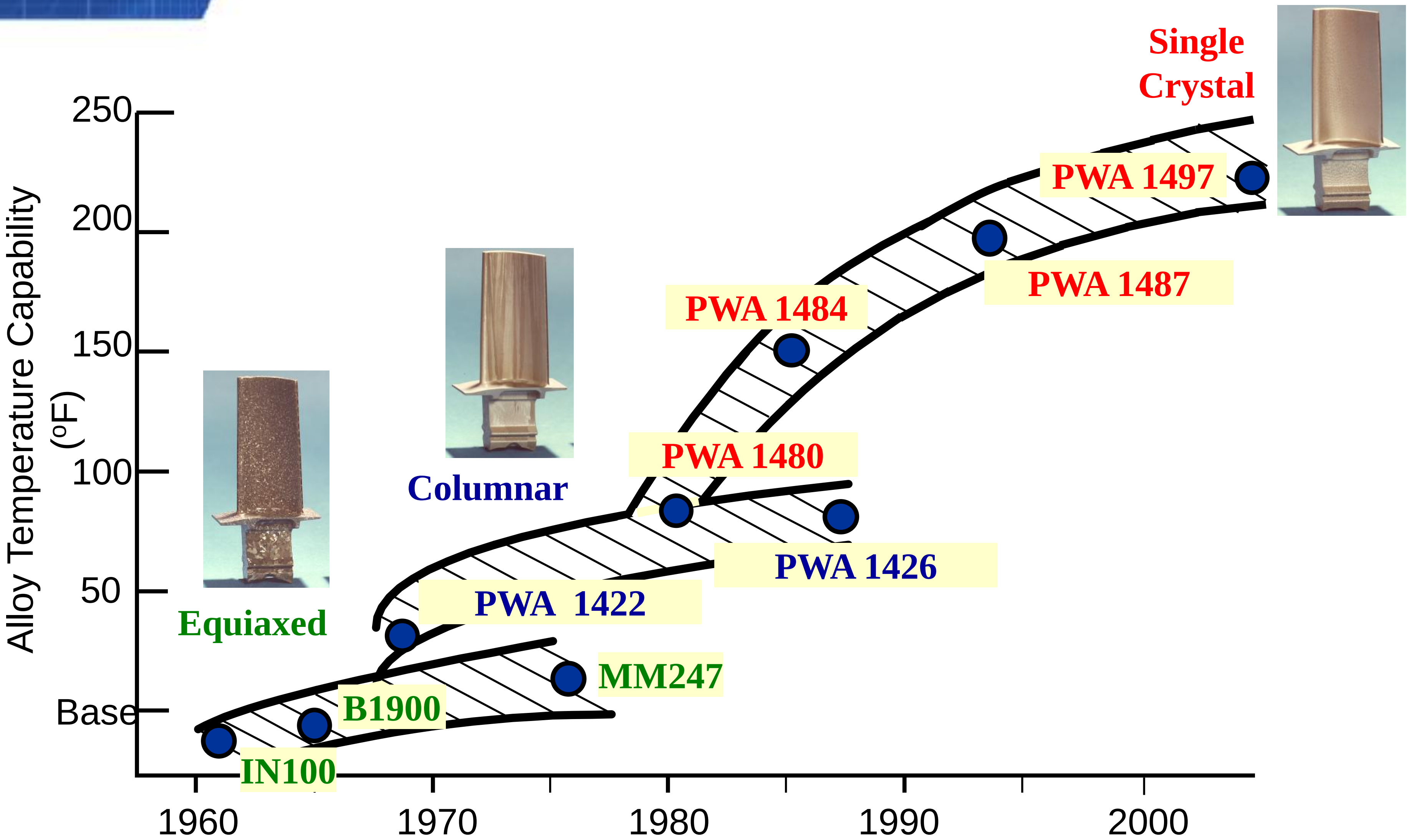
2nd Gen SC blades, Aluminide coatings, 2nd Gen PM/fracture tolerant disk

LFW Ti IBR, Dual Property Ni Disk, TBC blades, Burn resistant Ti, CatArc Metallic Coatings

Dual Property 3rd Gen PM disk, High modulus blade, 2nd Gen TBC coating

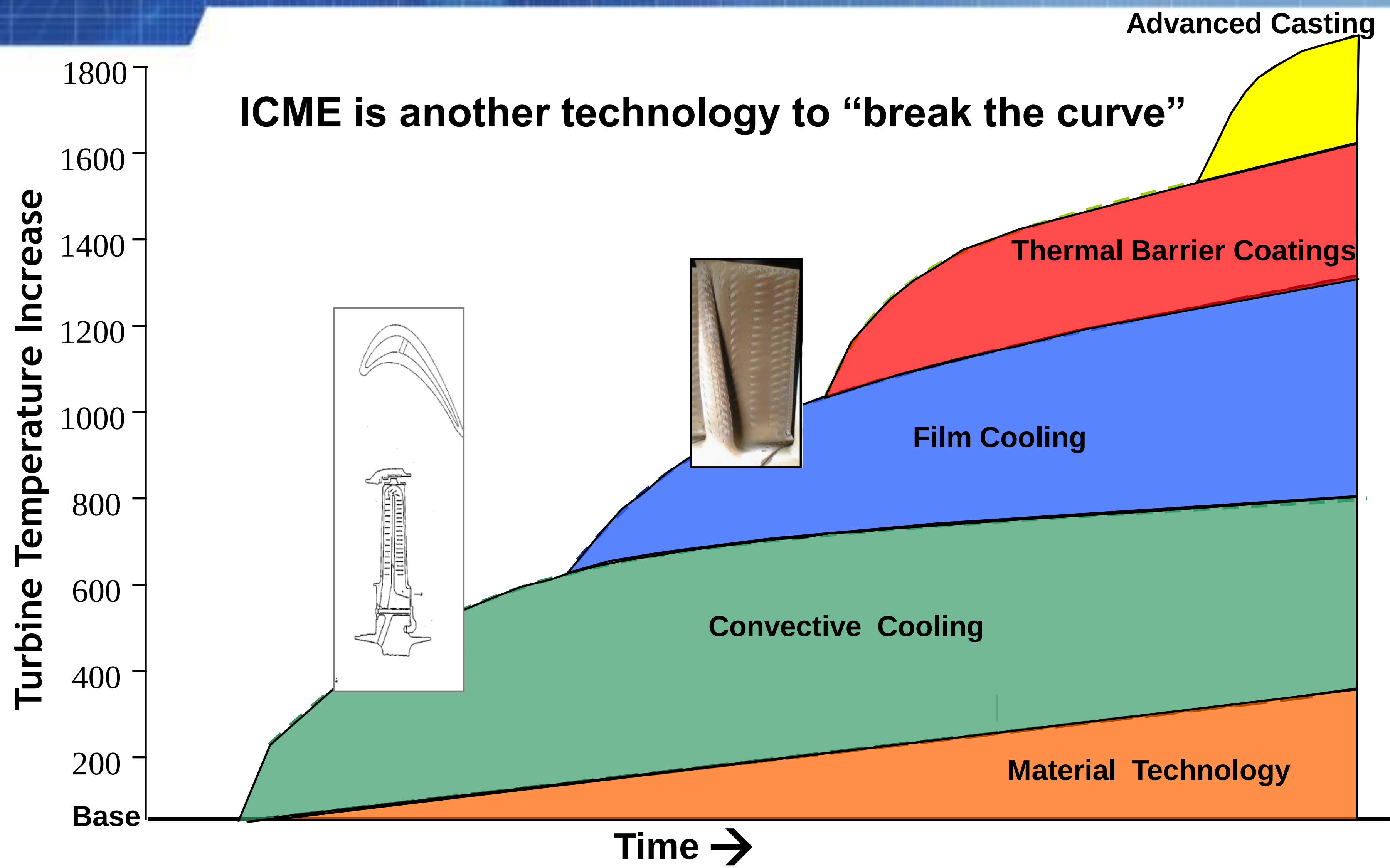
4th Gen PM disk alloy, Hybrid metallic airfoils, 3rd Gen TBC

Ni Superalloy Turbine Airfoils: Significant Advances in Alloys and Casting Processes



Not subject to the EAR per 15 C.F.R. Chapter 1, Part 734.3(b)(3)

Key Technology Advances for Turbine Airfoil Materials



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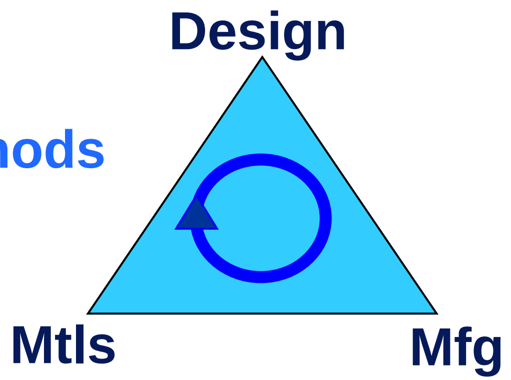
Materials & Product Engineering

<u>*Mechanical Properties*</u> *= fn (chemistry and microstructure)*

<u>*Microstructure*</u> *= fn (chemistry and processing)*

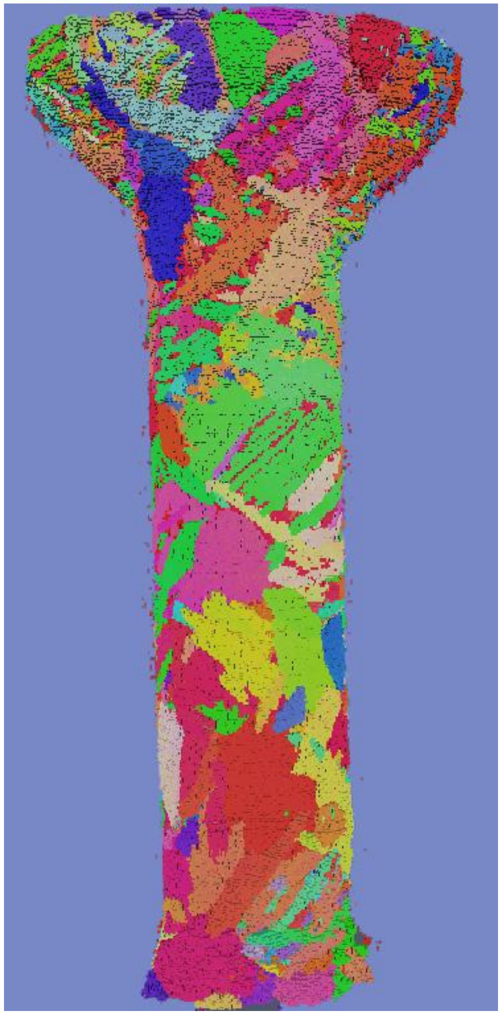
<u>*Processing*</u> *= fn (component geometry)*

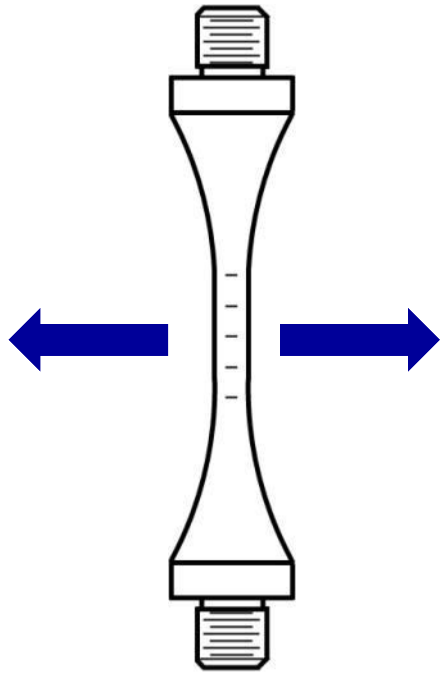
Materials, Manufacturing Methods and Component Design are Strongly Coupled



ICME -Integrated Computational Materials Engineering

What a Tensile Test Looks Like…..





MIL-HBK-5H

Table 5.4.1.0(b). Design Mechanical and Physical Properties of Ti-6Al-4V Sheet, Strip, and Plate

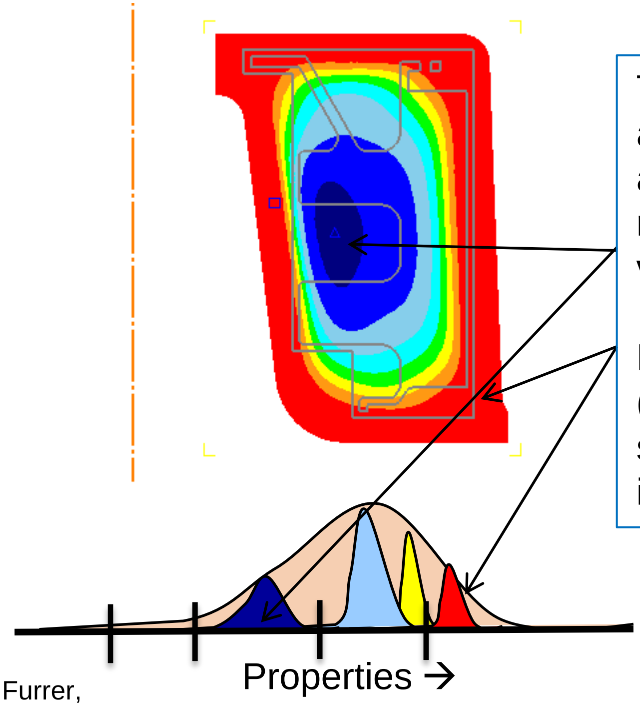
Specification	AMS 4911 and MIL-T-9046, Comp. AB-1					MIL-T-9046, Comp. AB-1			
Form	Sheet		Plate			Sheet, strip, and plate			
Condition	Annealed					Solution treated and aged			
Thickness, in.	≤ 0.1875		0.1875-2.000		2.001-4.000	≤ 0.1875	0.1875-0.750	0.751-1.000	1.001-2.000
Basis	A	B	A	B	S	S	S	S	S
Mechanical Properties:									
F_{tu}, ksi:									
L	134	139	130[a]	135	130	160	160	150	145
LT	134	139	130[a]	138	130	160	160	150	145
F_{ty}, ksi:									
L	126	131	120	125	120	145	145	140	135
LT	126	131	120[a]	131	120	145	145	140	135
F_{cy}, ksi:									
L	133	138	124	129	124	154	150	145	...
LT	135	141	130	142	130	162	...	...	...
F_{su}, ksi	87	90	79	84	79	100	93	87	...
F_{bru}, ksi:									
(e/D = 1.5)	213[b]	221[b]	206[b]	214[b]	206[b]	236	248	233	...
(e/D = 2.0)	272[b]	283[b]	260[b]	276[b]	260[b]	286	308	289	...
F_{bry}, ksi:									
(e/D = 1.5)	171[b]	178[b]	164[b]	179[b]	164[b]	210	210	203	...
(e/D = 2.0)	208[b]	217[b]	194[b]	212[b]	194[b]	232	243	235	...
e, percent (S-basis):									
L	8[c]	...	10	...	10	5[d]	8	6	6
LT	8[c]	...	10	...	10	5[d]	8	6	6
E, 10^3 ksi	16.0								
E_c, 10^3 ksi	16.4								
G, 10^3 ksi	6.2								
μ	0.31								
Physical Properties:									
ω, lb/in.^{3}	0.160								
C, K, and α	See Figure 4.5.1.0								

a The rounded T_{99} values are higher than specification values as follows: F_{tu}(L) = 131 ksi, F_{tu}(LT) = 132 ksi, and F_{ty}(LT) = 123 ksi.
b Bearing values are "dry pin" values per Section 1.4.7.1.
c 8%—0.025 to 0.062 in. and 10%—0.063 in. and above.
d 5%—0.050 in. and above; 4%—0.033 to 0.049 in. and 3%—0.032 in. and below.

To a Materials Engineer

To a Mechanical Engineer

Materials Capability Definitions



True material capability and property distributions are controllable and reproducible; not "random variability".

Properties are a fn (chemistry, microstructure, stain, cooling rate, etc.); i.e. pedigree.

From D.Furrer, OPTIMoM Conf., 2010

Materials properties are path dependent and are often "location-specific". Engineering specifications often treat entire material volume as single, homogeneous property capabilities.

Modeling and simulation can help enhance component property capability definitions

Traditional Materials Definitions

- Design Curves – Empirical; Data Driven
- Specifications
- Prints Notes
- Fixed Process Requirements

Requires Defining Material Equivalency and Methods to Differentiate Material of One Control Pedigree from Another

The Challenge: Need Models and Computational Infrastructure

Current materials definitions for design limit design flexibility and final component capabilities

There is a need for:

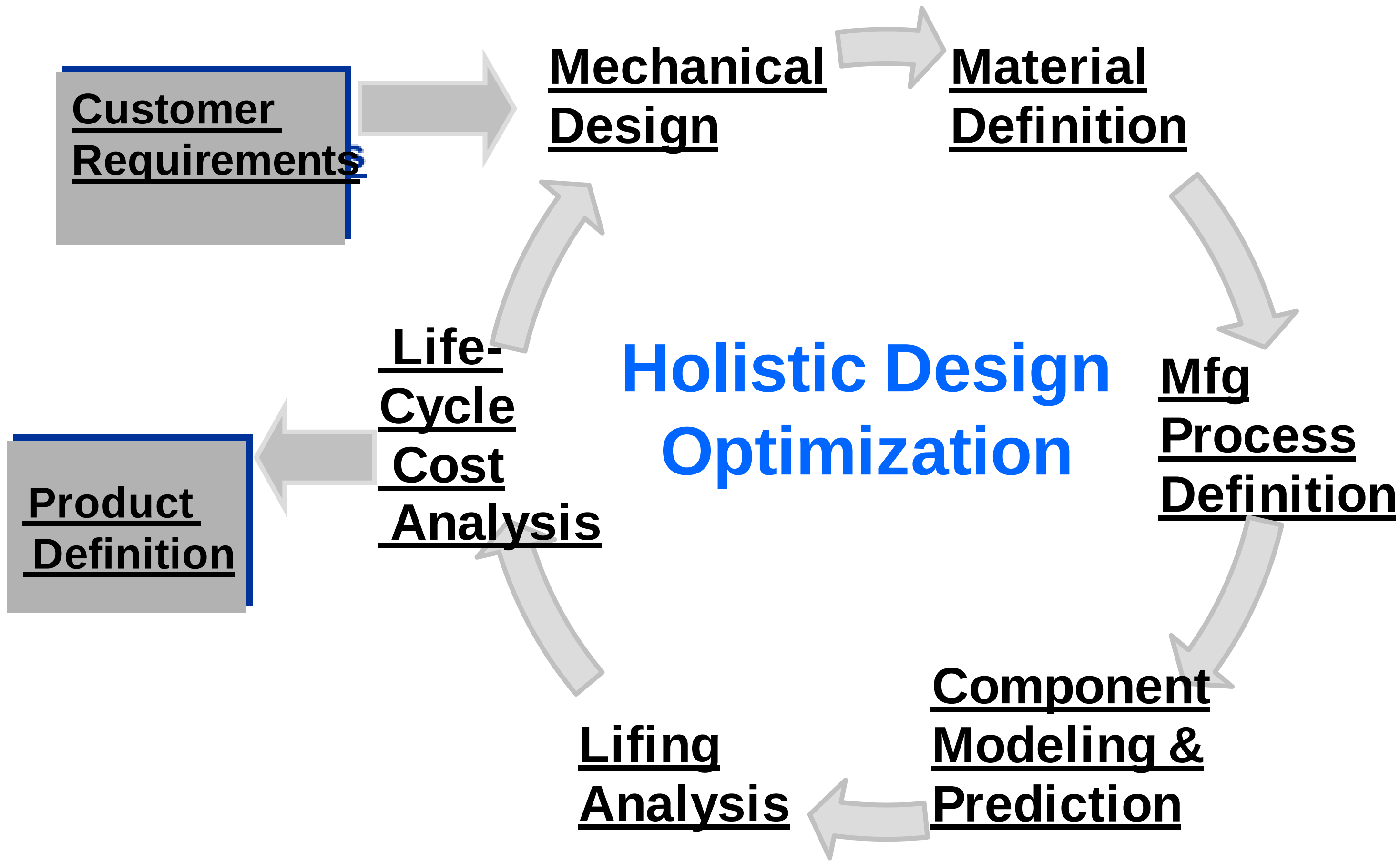
Model-Based Materials Definitions

Model-based material definitions enable location-specific prediction, analysis and optimization

Model-based materials definitions enable greater material, process and component definitions

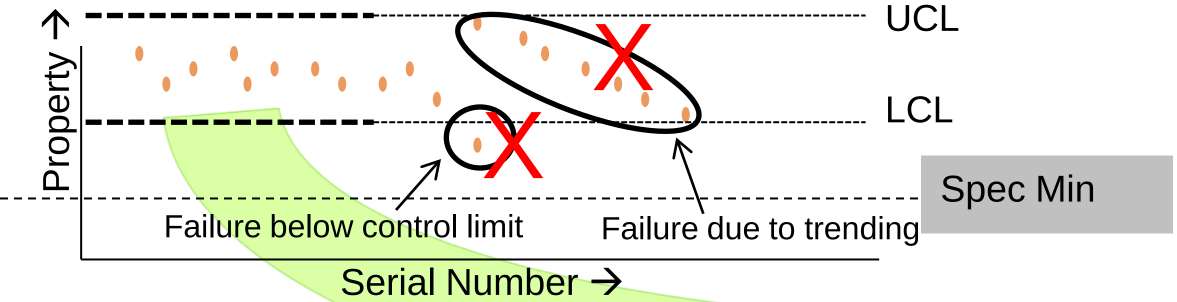
Goal is prediction and control of capabilities

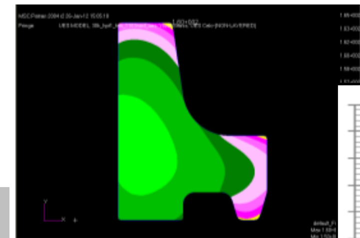
ICME Involved Linkage with Other Discipline Activities



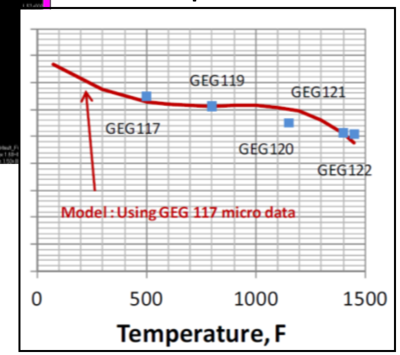
Materials Technology Enablers

Computational Models and Advanced Data Management





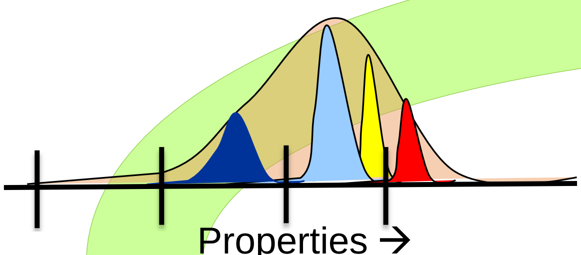
Predicted Material Properties



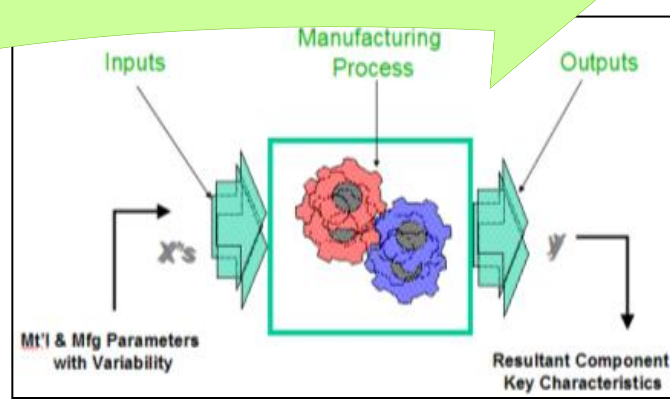
Capture of developmental and production data to support model development

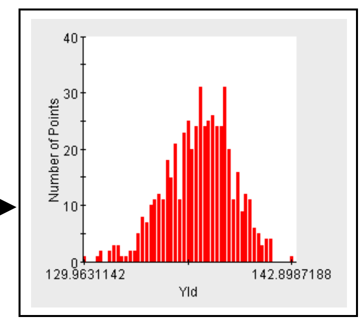
Goal is prediction and control of capabilities

Predicted Material and Component Properties



Traditional empirical property measurement and analysis migrating to materials models





Predicted Property Variability

Material & Process Modeling Goals

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- Develop Simulation Tools that Emulate Reality
- Develop Analytical Tools that Provide Insight in Material - Process - Property Relationships
- Implement Tools for Design and Manufacturing Benefits
  - Model-based Decisions
  - Tangible Improvements obtained based on Decisions

Holistic Integration: Digital Thread

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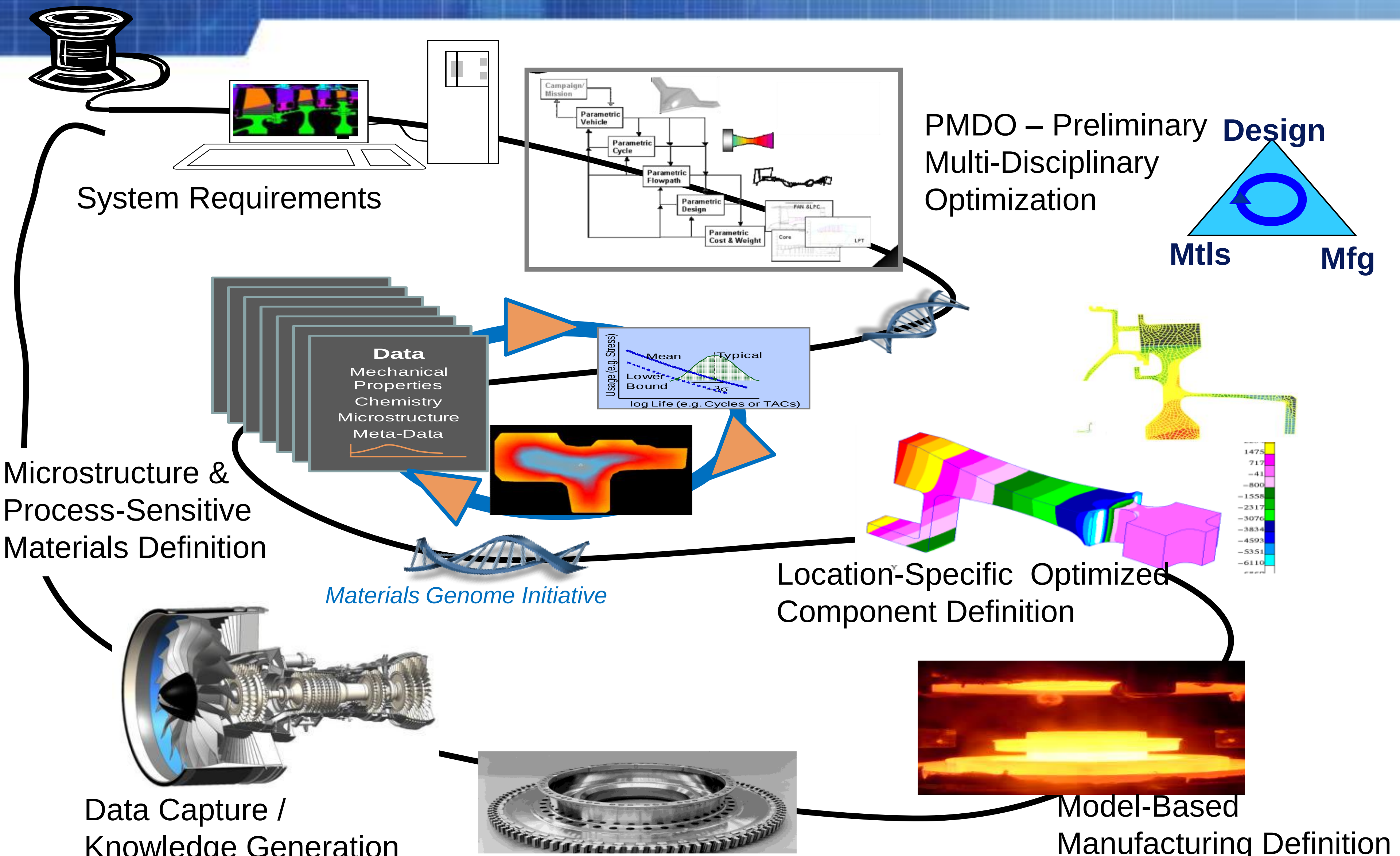
Example of Integrated Computational Materials & Mfg Engineering



Example of ICME Application

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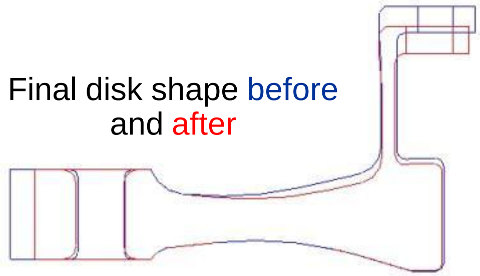
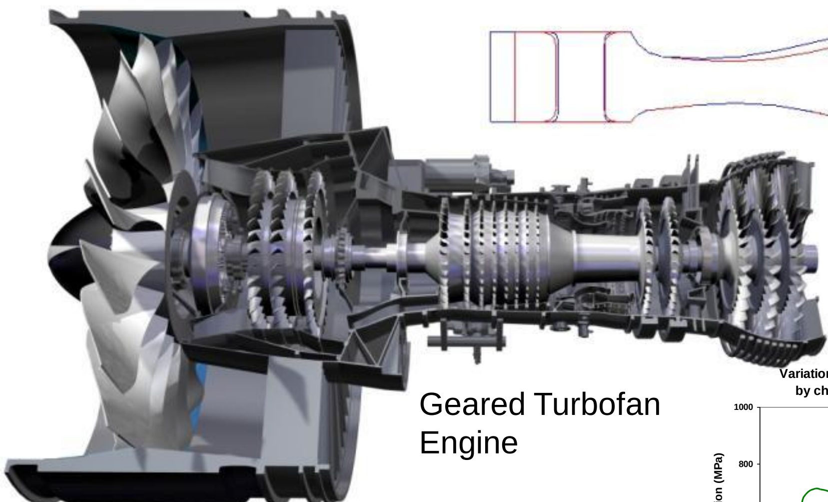
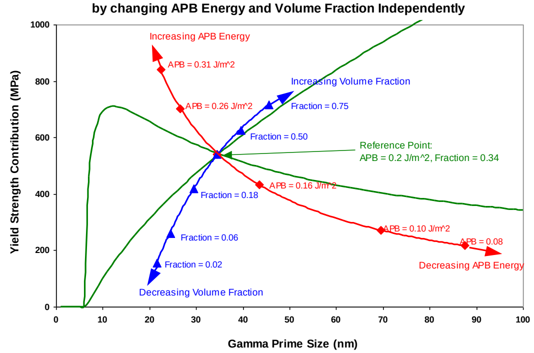




Geared Turbofan Engine

- Feasibility of full design integration demonstrated
  - Over 600 design loop runs with coupled part geometry and material capability driving design evolution
  - Realistic case studies

$$\sigma_{ys} = \underbrace{f_p\left\{\sigma(T)_{Ni3Al} + \sum_i\left(\frac{d\sigma}{dC_i}C_i\right)\right\}}_{\text{Yield of Primary } \gamma'} + \underbrace{M(1-f_p)0.43Gb\frac{\left(f_s/1-f_p\right)^{1/2}}{d}\left(\frac{2.56d\Gamma_{APB}}{Gb^2}-1\right)^{1/2}}_{\text{Shearing of Secondary } \gamma' \text{ (Pairs)}}$$
$$+\underbrace{Mf_t\left\{\frac{\Gamma_{APB}}{b}\right\}}_{\text{Shearing of Tertiary } \gamma'} + \underbrace{f_\gamma\left(\frac{T_o}{T}\right)\left\{\sum_i\frac{d\sigma}{dC_i^{1/2}}C_i^{1/2}\right\}}_{\gamma \text{ Solid Soln Strengthening}} + \underbrace{(1-f_p)k_y^{\gamma}d^{-1/2}}_{\text{Hall-Petch } \gamma \text{ Phase}} + \underbrace{f_pk_y^{\gamma'}d^{-1/2}}_{\text{Hall-Petch Primary } \gamma'}$$



Cost Benefit

System Benefits

>50% Reduction in Design Cycle Time

Case Study	Heat Treat	Forging	Part	Forge Wt	Part Wt	Burst Speed	Comments
1	Constant	Variable	Variable	-18%	-15%	+6%	Current State of the Art
2	Variable	Variable	Constant	-11%	n/a	+12%	Final Part shape constrained
3	Variable	Variable	Variable	-21%	-19%	+19%	Full impact of tool

Disciplines Touched by ICMSE

Integration of Computational Materials Science and Engineering is Complicated

- Materials
- Manufacturing
- Design
- Structures
- Quality
- Supply-Chain

Challenges to Effective ICME Deployment

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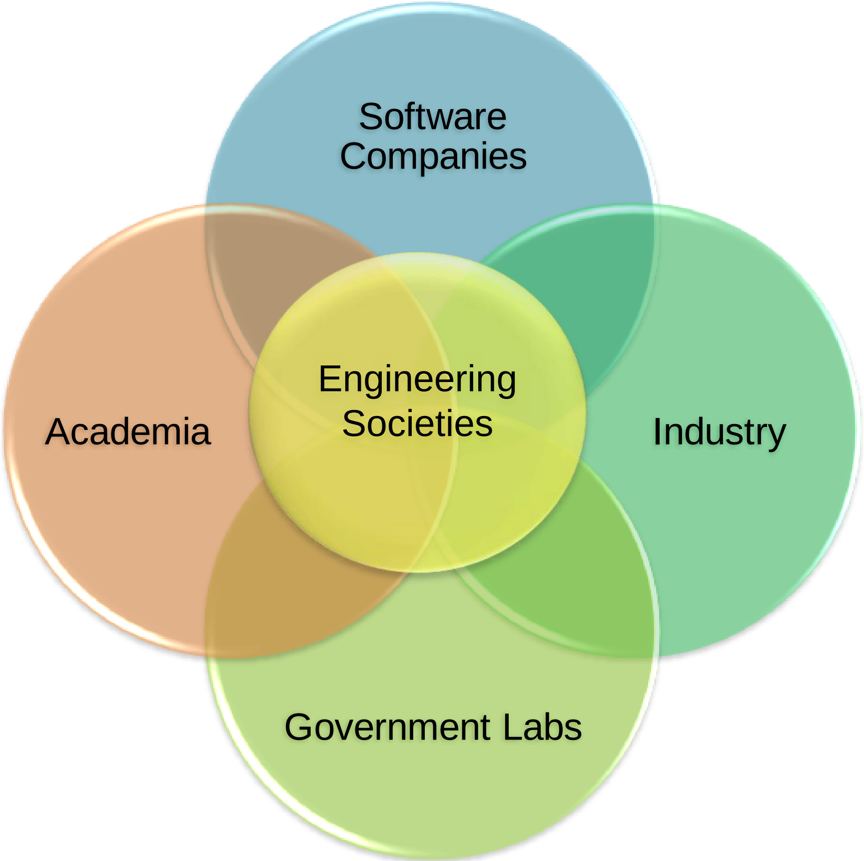
- Accurate computational models
- Efficient simulation software tools
- Data and databases for model application
- Industry standard methods and protocols
- Computational methods for design linkages
- Well trained interdisciplinary workforce

Unique engineering skill sets are required to support each challenge

Computational Supply-Chain

A series of well-established, capable and viable organizations that provide necessary portions of the ICME Value Chain

- Fundamental Model Development
- Model Integration into Software Packages
- Maintenance of Software Tools
- Database Generation
- Application Engineering
- Customer Approval and Certification
- Education and Training



Conclusions

- ICME: Potential for dramatic changes to development time, cost, and product capabilities
- Computational materials engineering enables virtual manufacture and component testing for optimization and risk mitigation
- Application of ICME has several challenges: trained practitioners; tools and methods; and computational infrastructure

Any Questions?